

## Introduction

Scientific databases are becoming critical to research in the industrial and academic communities. The NIST Workshop on Crystallographic Databases was one in a series of NIST sponsored workshops each focusing on a particular type of data including, among others, crystallographic, thermodynamic, phase diagram, and mass spectral data. By bringing together top scientists involved in producing crystallographic data with users of the resulting databases, this Workshop served as a forum to examine how well the needs of the scientific community are being met and what data activities the community feels are important in the future. During the Workshop, three sessions of scientific presentations were held—(1) Formal Data Activities; (2) Scientific Uses of the Databases; and (3) Data Transfer: ensuring state of the art technology. In the first session, a representative from each of the data centers covered present activities and projected future activities of their data center. In the second session, the focus was on using crystallographic databases in analysis, in the prediction of materials properties and in the design of new chemicals, pharmaceuticals, and materials. In the third session, speakers addressed issues related to data transfer such as data exchange standards, the role of journals in the evaluation of published data, data exchange between the journals and crystallographic data centers, and computerized modes of data dissemination.

Following the presentations, a discussion session focused on Barriers to the Use of Crystallographic Data and on Partnerships for the Future. After the Workshop, the speakers submitted manuscripts which are published in this issue of the NIST Journal of Research. Following these papers are highlights of the discussion session.

As anticipated, the Workshop was attended by a diverse group who use crystallographic data in their research or are involved with this data in some other capacity, such as managers of scientific projects, journal editors, on-line system designers, instrument manufacturers, and librarians, among others. The Workshop revealed that the users of crystallographic data are being well served. The Data Centers have built evaluated databases covering all classes of compounds and they have developed theories and scientific programs for standardizing, evaluating and searching the data. Nevertheless, the topics addressed herein clearly demonstrate that the data field is in a period of dynamic transition that is being driven by many factors including a greatly increased user demand for information. Many attendees commented that the Workshop was both instructive and useful, and that it should be repeated in a few years.

The Workshop was held on August 29–30, 1995 on the campus of the National Institute of Standards and Technology (NIST) in Gaithersburg, Maryland, with the Standard Reference Data Program (SRDP) acting as host. The Workshop had no external funding, and NIST's support was fundamental to its success. We are particularly grateful to Dr. John R. Rumble, Jr., Chief of SRDP, whose support was critical for making this Workshop happen. Likewise, we appreciate the suggestions and assistance of Jean Gallagher, Sabina Crisen, and other SRDP staff members.

Many scientists contributed to the Workshop and this publication. We sincerely thank the following—David G. Watson (Cambridge Crystallographic Data Centre), Carolyn P. Brock (University of Kentucky), and Brian McMahon (International Union of Crystallography) for organizing excellent and timely sessions and for their assistance in editing the manuscripts that appear in this issue of the NIST Journal of Research; and Judith Flippen-Anderson (Naval Research Laboratory) and the attendees for a thoughtful and productive discussion session.

**Vicky Lynn Karen**  
**Alan Mighell**  
Special Issue Editors